Patent Claims

1. Laser-compatible NIR marker dyes based on polymethine, containing substituted derivatives of benzooxazole, benzothiazole, 2,3,3trimethylindolenine, 2,3,3-trimethyl-4,5-benzo-3H-indolenine, 2- and 4-picoline, lepidine, chinaldine and 9-methylacridine of the general formula la or lb or lc

$$R^4$$
 R^5
 R^3
 R^2
 R^1
 R^3

$$R^3$$
 R^5
 R^2
 R^1
 R^5

where Z is

$$\begin{array}{c}
R^{12} \\
R^{7} \\
R^{8}
\end{array}$$

or

or

or

or



- X or Y is an element from the group comprising O, S, Se or the structural element N-alkyl or C(alkyl)₂,
 - n represents the numerical value 1, 2 or 3,
- R¹ R¹⁵ are identical or different and can be hydrogen, one or more alkyl- or aryl-, heteroaryl- or heterocycloaliphatic groups, a hydroxy or alkoxy group, an alkyl-substituted or cyclic amine function and/or two *ortho* groups, e.g., R² and R³, together can form another aromatic ring,
- at least one of the substituents R^1 R^{15} can be an ionizable or ionized substituent such as SO_3^- , PO_3^- , COO^- or NR_3^+ which determines the hydrophilic characteristics of these dyes,
- at least one of the substituents R¹ R¹⁵ can represent a reactive group which enables a covalent linking of the dye with the carrier molecules mentioned above, and
- U-V or U'-V' are identical or different and can comprise hydrogen, a saturated aliphatic, heteroaliphatic or a lactone or thiolactone grouping.
- 2. Laser-compatible NIR marker dyes according to claim 1, characterized in that the reactive group is selected from the following functionalities: isothiocyanates, monochlorotriazines, dichlorotriazines, aziridines, sulfonyl halides, *N*-hydroxysuccinimide ester, imido esters, glyoxal or aldehyde for amine and hydroxy functions or maleimides or iodacetamide for thiol functions and phosphoramidites for labeling DNA or RNA or fractions thereof.
- 3. Laser-compatible NIR marker dyes according to claim 1, characterized in that the reactive group is bonded to the actual chromophore via spacer groups of the general structure $-(CH_2)_m$ -, wherein m can have values from 1 to 18.
- 4. Laser-compatible NIR marker dyes according to claim 1, characterized in that the structural unit =CR⁷- also contains a bridge over four-, five-

and six-member ring systems, wherein reactive groups are also located at the latter and substituents A-G can have the same functionality as substituents R¹-R¹⁵.

5. Laser-compatible NIR marker dyes according to claim 4, characterized in that the structural unit = CR^7 - (n = 2) represents

$$\bigwedge_{A_{\Theta}}^{B}$$

6. Laser-compatible NIR marker dyes according to claim 4, characterized in that the structural unit = CR^7 - (n = 2) represents

$$C$$
 A_{Θ}

7. Laser-compatible NIR marker dyes according to claim 4, characterized in that the structural unit = CR^7 - (n = 3) represents

$$\bigcup_{E}^{D}$$

8. Laser-compatible NIR marker dyes according to claim 4, characterized in that the structural unit = CR^7 - (n = 3) represents

$$\bigcup_{E \to G}^{D}$$

- 9. Laser-compatible NIR marker dyes according to claim 4, characterized in that substituents A-C represent O, S, C(CN)2 or N-R, wherein R in N-R can represent an aliphatic or aromatic or reactive aliphatic or aromatic group such as $(CH_2)_n COOH$ or $(CH_2)_n NH_2$.
- 10. Laser-compatible NIR marker dyes according to claim 4, characterized in that substituent D represents Cl or an aromatic or aliphatic ring system on which reactive substituents corresponding to R¹ to R¹⁵ are possibly arranged.



- 11. Laser-compatible NIR marker dyes according to claims 1 to 10, characterized in that they are used for optical labeling of proteins, nucleic acids, oligomers, DNA, RNA, biological cells, lipids, polymers, drugs or polymer particles.
- 12. Method for qualitative or quantitative determination of proteins, nucleic acids, oligomers, DNA, RNA, biological cells, lipids, polymers, drugs or polymer particles, characterized in that the functional groups of the laser-compatible NIR marker dyes are covalently linked to an OH-, NH₂- or SH-function of the substances to be determined.
- 13. Method according to claim 12, characterized in that the coupling reaction is carried out in aqueous solution.